

A SIMPLE MODEL FOR REGENERATION OF A POLYMERIC SORBENT SATURATED WITH PHENOL

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Abstract—Regeneration of spent resin particles is a crucial step in a cyclic adsorption process for removal of phenolic species from wastewater. A simple model is developed for simulating the regeneration behavior in finite batch adsorbers. It is then applied to the regeneration by sodium hydroxide solutions, of a polymeric sorbent, SP206, saturated with phenol. Analytic solutions of the model are obtained based on both the reaction front assumption and the quasi-steady state approximation in the resin particle, considering the fact that sodium hydroxide reacts with phenol very quickly.

Key words: Regeneration of Spent Resin, Removal of Phenol, Analytic Solutions, Batch Operation

INTRODUCTION

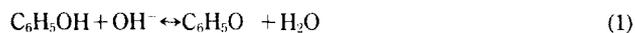
Phenol and its derivatives formed by chemical reactions, can impart an objectionable taste or odor, but a more serious problem is that these substances are known to be potentially carcinogenic and mutagenic [1]. Activated carbon has been used as a common adsorbent in treating drinking waters so far, but there is a weak point in its application in that there is a considerable amount of irreversible adsorption. The regeneration of spent carbon is not easy and even if possible, an expensive task. Furthermore, the disposal of spent carbon causes secondary environmental pollution. Thus the use of polymeric sorbents has drawn attention as an alternative to activated carbon processes for wastewater treatment.

Adsorption processes are usually carried out in a cyclic way which involves three consecutive steps: saturation (or adsorption), regeneration (or desorption), and washing. Among these three steps, the regeneration step is crucial when optimizing the overall adsorption process [2]. When Costa and Rodrigues [3] reported the promising application of polymeric sorbents, we decided to start our own research [4, 5]. They used a polystyrene-based polymeric sorbent crosslinked with divinylbenzene to remove phenol from aqueous solutions. The sorbent particle saturated with phenol was regenerated by sodium hydroxide solutions. In a series of publications [6-8], they developed rigorous models for the regeneration step in CSTR and fixed-bed adsorbers and further simulated regeneration behavior for CSTR and fixed-bed operations by using their models based on an assumption of the reaction front in the particle.

It is not a trivial matter from the practical point of view to develop a promising theoretical model which is simple but still accurate enough. For such a theoretical model to be used successfully under various operational conditions, the first essential condition is to obtain results in the shortest time possible. This condition leads usually to a serious compromise between the intention to accept a realistic physical feature and the desire to cut

computation time [9, 10].

In this work, we suggest quite a simple model for the regeneration of a resin sorbent, SP206, saturated with phenol when sodium hydroxide is used as a regenerant. When a polymeric sorbent saturated with phenolic species is regenerated by using hydroxide solutions, the following reaction takes place inside the sorbent and in the bulk solution



This reaction is very fast and nearly irreversible. If it is assumed that the phenol molecules adsorbed are stationary in the resin and the pore diffusion of hydroxide is the major rate-controlling step, the reaction will occur entirely at a reaction front which penetrates into the particle as a shock transition. Phenate, which is formed by the reaction, diffuses out quickly from the resin matrix because of the Donnan potential effect [6]. Under various conditions of the regeneration process, several analytical solutions of the model are obtained by assuming the reaction front and the quasi-steady state concentration profile in the sorbent particle. Such solutions can be used extensively in simulating the regeneration behavior of spent resins in a batch adsorber.

THEORETICAL

1. Equilibrium Relationships

The equilibrium constant for the reaction between phenol and sodium hydroxide Eq. (1), at 20°C is [6]

$$K_{eq} = \frac{C_{PN}}{C_P C_S} = 13\text{m}^3/\text{mol} \quad (2)$$

where C_{PN} , C_P and C_S are the concentrations of phenate, phenol and hydroxide species, respectively. It was also found that the adsorption isotherm of phenol on SP206 follows the Langmuir equation [4],

$$Q_p = \frac{Q_m b C_P}{1 + b C_P} \quad (3)$$

where Q_p is the adsorbed phenol concentration expressed in

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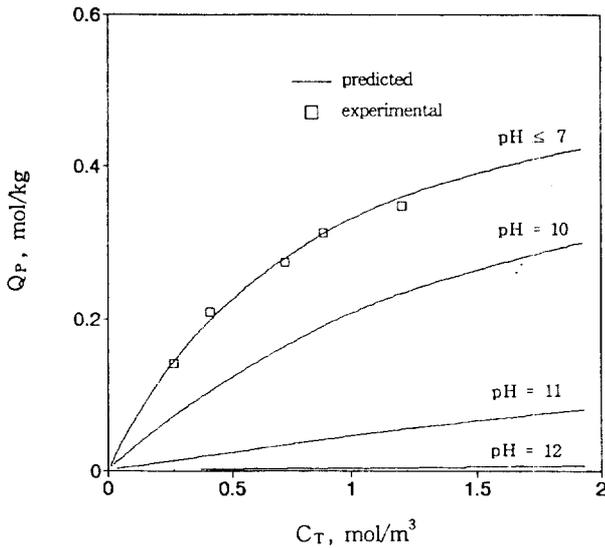


Fig. 1. Effect of pH on isotherm of phenol on SP206 at 20°C (Phenol/SP206).

mol/kg-dry sorbent. For a system, phenol/SP206, the Langmuir parameters, Q_m and b , were determined to be 0.626 mol/kg and 1.136 m³/mol, respectively, by fitting experimental data to the Langmuir equation [4].

The total molar concentration of phenol and phenate in the solution is

$$C_T = C_P + C_{PX} \quad (4)$$

Combining Eqs. (2)-(4) together, we get

$$Q_P = \frac{Q_m b C_P}{1 + K_{eq} C_S + b C_T} \quad (5)$$

The effect of pH (or C_S) on adsorption equilibrium of phenol can be easily predicted by Eq. (5) [6]. Fig. 1 shows isotherms of phenol at various pH values, which are predicted from an experimental isotherm measured at pH=7. This figure shows that the effect of pH is very critical for pH values higher than 7 and the sorbent can uptake only a little amount of phenol at pH values over 12.

2. Modeling

When the reaction between phenol and sodium hydroxide occurs at the reaction front, R_r , at any instant and the pore diffusion of hydroxide is the major rate-controlling step, the concentrations of phenate and hydroxide in the batch adsorber can be represented by their mass balance equations.

For phenate,

$$\frac{dC_{PX}}{dt} = -\frac{3wQ_P}{VR_0^3} R_r^2 \frac{dR_r}{dt} \quad (6)$$

For hydroxide,

$$\frac{dC_S}{dt} = \frac{3wQ_P}{VR_0^3} R_r^2 \frac{dR_r}{dt} - \frac{w\varepsilon_P}{\rho_P V} \frac{d\bar{c}_S}{dt} \quad (7)$$

where V is the volume of the solution in the batch and w is the weight of sorbent particles charged. ε_P and ρ_P are the particle porosity and density, respectively. The last term of Eq. (7) represents the change of hydroxide concentration in the pore space of resin particles. The average concentration of hydroxide in the

particle, \bar{c}_S , can be calculated from its concentration profile as follows:

$$\bar{c}_S = \frac{3}{R_0^3} \int_{R_f}^{R_0} R^2 c_S dR \quad (8)$$

When the reaction front penetrates into the sorbent particle as a shock transition, the transfer rate through the particle over the reacted outer region, $R_f \leq R \leq R_0$, may be assumed to be independent of radial positions, since the reaction takes place only at R_r . This assumption is called "quasi-steady state approximation" [11]. Thus, the transfer rate at R may be given by a function of time, $H(t)$.

$$H(t) = 4\pi R^2 \varepsilon_P D_P \frac{\partial c_S}{\partial R} \quad R_f \leq R \leq R_0 \quad (9)$$

Eq. (9) should satisfy the following conditions,

$$c_S = 0 \quad \text{at } R = R_f \quad (10)$$

$$\varepsilon_P D_P \frac{\partial c_S}{\partial R} = k_f \{C_S(t) - c_S\} \quad \text{at } R = R_0 \quad (11)$$

where k_f is the film mass transfer coefficient of hydroxide and $C_S(t)$ is the bulk concentration of hydroxide at a time, t . Furthermore a condition at $R = R_f$ can be applied to evaluate the variation of the reaction front in terms of time:

$$\varepsilon_P D_P \frac{\partial c_S}{\partial R} \Big|_{R_f} = -\rho_P Q_P \frac{\partial R_r}{\partial t} \quad (12)$$

Eq. (12) implies that the reacted amount of phenol at any instant in time is equal to the amount of hydroxide transferred to the reaction front by pore diffusion. Integrating Eq. (9) over R at a given time and applying two conditions, Eqs. (10) and (11), yields the concentration profile of hydroxide in the particle at a given time:

$$c_S(R, t) = \frac{R_0^2 (R - R_f) k_f}{[\varepsilon_P D_P R_f^2 + R_0 (R_0 - R_f) k_f]} C_S(t) \quad (13)$$

The variation of the reaction front can be obtained by inserting the derivative of $c_S(R, t)$ with respect to R at $R = R_f$ into Eq. (12):

$$\frac{\partial R_r}{\partial t} = \frac{-\varepsilon_P D_P R_0^2 k_f / \rho_P Q_P}{\varepsilon_P D_P R_f^2 + R_0 R_f (R_0 - R_f) k_f} C_S(t) \quad (14)$$

3. Analytic Solution

Eqs. (6)-(8), (13) and (14) can be written into the following dimensionless form after some manipulation:

$$Y_{PX}(\tau) = -\alpha(x^3 - 1) \quad (15)$$

$$Y_S(\tau) = 1 + \alpha(x^3 - 1) - \beta \bar{y}_S(\tau) \quad (16)$$

$$\bar{y}_S(\tau) = 3 \int_{x_f}^1 x^2 y_S(x, \tau) dx \quad (17)$$

$$y_S(x, \tau) = \frac{\left(1 - \frac{x_f}{x}\right)}{1 - (1 - 1/Bi)x} Y_S(\tau) \quad (18)$$

$$\frac{\partial x_f}{\partial \tau} = -\frac{1}{x_f [1 - (1 - 1/Bi)x_f]} Y_S(\tau) \quad (19)$$

Here, the dimensionless variables are defined as

$$\alpha = \frac{wQ_P}{VC_S^0} \quad (20)$$

$$\beta = \frac{w\varepsilon_P}{\rho_P V} \quad (21)$$

$$Bi = \frac{k_f R_0}{\varepsilon_P D_P} \quad (22)$$

$$\tau = \frac{D_P}{R_0^2} \frac{\varepsilon_P C_S^0}{\rho_P Q_P} t \quad (23)$$

$$x = \frac{R}{R_0}, \quad x_f = \frac{R_f}{R_0} \quad (24)$$

$$Y_s = \frac{C_S}{C_S^0}, \quad y_s = \frac{c_s}{C_S^0}, \quad Y_{PN} = \frac{C_{PN}}{C_S^0} \quad (25)$$

Here α is the capacity factor for an individual test, which represents the ratio of the amount of phenol preadsorbed on the resin to the initial amount of regenerant [9]. β is the volume ratio, between the pore space of resin particles and the volume of bulk solution. From Eqs. (17) and (18), we get

$$\bar{y}_s(\tau) = \frac{(2 - 3x_f + x_f^3)}{2[1 - (1 - 1/Bi)x_f]} Y_s(\tau) \quad (26)$$

Combining Eqs. (16) and (26) yields

$$Y_s(\tau) = \frac{1 + \alpha(x_f^3 - 1)}{1 + \frac{\beta(2 - 3x_f + x_f^3)}{2[1 - (1 - 1/Bi)x_f]}} \quad (27)$$

Finally, Eq. (19) becomes

$$\frac{\partial x_f}{\partial \tau} = - \frac{1 + \alpha(x_f^3 - 1)}{x_f \left[(1 + \beta) - \left(1 + \frac{3\beta}{2} - \frac{1}{Bi} \right) x_f + \frac{\beta}{2} x_f^3 \right]} \quad (28)$$

Eq. (28) can be analytically integrated from $x_f=1$ to any x_f . We then get

$$\begin{aligned} \tau = & \frac{\beta}{4\alpha} (1 - x_f^2) \\ & + \frac{BG}{6\alpha^2} \left[\sqrt{3} \left\{ \tan^{-1} \left(\frac{-1 + 2B}{\sqrt{3}} \right) - \tan^{-1} \left(\frac{-1 + 2Bx_f}{\sqrt{3}} \right) \right\} \right. \\ & \left. + \ln \left\{ \frac{(1 + Bx_f)(1 - B + B^2)^{1/2} (1 - \alpha + \alpha x_f^3)^2}{(1 + B)(1 - Bx_f + B^2 x_f^2)^{1/2}} \right\} \right] \quad (29) \end{aligned}$$

$$\text{where } B = \left\{ \frac{\alpha}{(1 - \alpha)} \right\}^{1/3} \quad (30)$$

$$G = 2\alpha - \beta + 3\alpha\beta \quad (31)$$

$$Z = \frac{\left(2 + 3\beta - \frac{2}{Bi} \right) \alpha}{(BG)} \quad (32)$$

For given values of α , β and Bi , the variation of x_f can be evaluated from Eq. (29). Once x_f is known, the concentrations of phenate and hydroxide may be calculated from Eqs. (15) and (16). The solution, Eq. (29), can be reduced to other simple forms by taking the limited values of α , β and Bi according to the condition under which we operate.

EXPERIMENTAL

The sorbent used in this study was a nonfunctional macroreticular polystyrene resin crosslinked with divinylbenzene, SP206, manufactured by Mitsubishi Co. The properties of this sorbent measured and obtained from the manufacturers' specifications are

Table 1. Properties of a polymeric sorbent SP206

Property	Value	Units
Particle size*	250/1000	μm
Particle density	640	kg/m^3
Packing porosity	0.44	-
Moisture content*	50	%
Surface area*	556	m^2/g
Average pore diameter*	70	\AA

*from manufacturers' specification.

listed in Table 1. The average particle diameter of the sorbent particles was estimated to be 0.50×10^{-3} m from microscopic measurement. All sorbent particles were leached with methanol to remove impurities and to wet internal pores prior to use. Sorbent particles were loaded in a 0.01 m ID glass column and a ten-bed volume of methanol was passed through the column at a flow rate of 1×10^{-6} m³/min. After leaching with methanol, a twenty-bed volume of distilled and deionized water (Sigma LC grade) was passed at the same flow rate in order to remove methanol. It was confirmed that methanol at the column effluent after passing a ten-bed volume of water was no longer detected by a flame ionization detector. Stock solution of phenol were made up by dissolving the reagent-grade chemical supplied by Sigma Chemical Co. into distilled and deionized water.

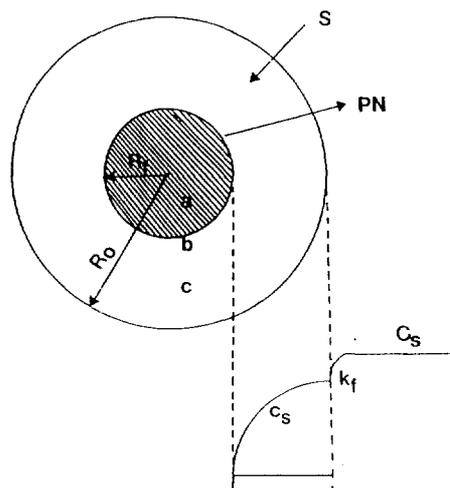
Equilibrium data were taken by introducing a given amount of sorbent into a mixed solution of 2×10^{-4} m³, shaking it in a constant temperature incubator at 20°C for a week and measuring the adsorbate concentrations remaining in the solution. A week was enough for the system to reach equilibrium. The dry-base weight of sorbent was measured by weighing after drying for 10 hours in a vacuum oven at 90°C.

Desorption experiments were conducted in a Carberry-type batch adsorber of 2×10^{-3} m³ used in previous studies [4]. Sorbent particles were loaded into four cages made of 80 mesh stainless-steel screen and the cages were affixed to the rotating shaft to permit good contact with the solution. All the experiments were carried out at approximately 500 rpm. Prior to desorption experiments, the charged resin particles in the cages were saturated with phenol solution in a batch adsorber and moved into a sodium hydroxide solution of known concentration. Since the reaction between phenol and hydroxide can take place in the whole fluid phase including particle pores, the operation should be done carefully to minimize a possible error from the amount of phenol attached on the surface of the cages. The phenol concentration on the resin phase was calculated from the material balance for the saturation step. The amount of phenol and phenate in the adsorber was measured by a UV spectrometer (Varian DMS 100S) at 272 nm which is an isobastic point of two species. Hydroxide concentration was measured by a pH meter (Fisher Model 420).

RESULTS AND DISCUSSION

1. Different Forms of Analytic Solutions

For a given set of conditions, we can calculate the time necessary for the reaction front to reach a radial position, x_f , from Eq. (29). It is also possible to obtain the value of x_f at any instant in time by using a trial and error procedure. Once x_f is known, calculation of the concentrations of phenate and hydroxide from Eqs. (15) and (16) is straightforward. The solution obtained here, Eq. (29), is a general solution for the film-pore diffusion model



- a : unreacted core
- b : reaction front
- c : reacted outer region
- (diffusion of hydroxide occurs)

Fig. 2. Schematic diagram showing a reaction front and concentration profiles.

that takes into account film mass transfer as well as pore diffusion under the reaction front assumption and the pseudo-steady state profile approximation. This kind of solution has been known to be very useful in various situations; reactions between gas and solid reactant which is impregnated in an inert porous medium [11], ion-exchanging reactions, irreversible adsorptions [12], and catalyst regeneration [11] etc. A common situation for all the cases mentioned above is that the reaction occurs very fast and the mass transfer is the rate-controlling step. In this case, a reaction front is formed inside the particle and it moves gradually to the center of the particle like a shock wave. Therefore this solution can be reduced to other simple forms by assuming specific conditions of the regeneration system. It is possible to consider four different cases:

- (1) $Bi \rightarrow \infty$
- (2) $\beta \rightarrow 0$
- (3) $Bi \rightarrow \infty$ and $\beta \rightarrow 0$
- (4) $Bi \rightarrow \infty$, $\beta \rightarrow 0$, and $Y_s = Y_s^0 (= 1.0)$

In the first case one neglects the film mass transfer resistance at the external surface of resin particles. In this case, the term, $1/Bi$, in Eq. (29) can be omitted. This implies that the inclusion of the effect of film mass transfer resistance does not give any complexity to the form of the analytical solution. The second case has a very small volume ratio, β . By letting β be zero, we get $G = 2\alpha$ and $Z = (1 - 1/Bi)/B$. This second solution is similar to that of Spahn and Schlunder [9]. For the third case, Z is further simplified as $1/B$. The most simple solution can be obtained in the final case which has a further assumption that the concentration of hydroxide in the bulk solution remains constant during the regeneration when $Bi = \infty$ and $\beta = 0$:

$$\tau = \frac{1}{6}(2x_f^3 - 3x_f^2 + 1) \tag{33}$$

The assumption of constant bulk concentration is very reason-

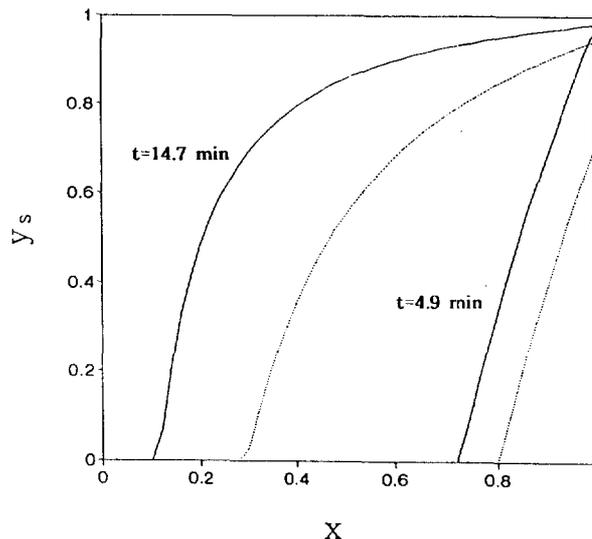


Fig. 3. Concentration profiles of hydroxide in the resin particle at different times.

(Run 1, — $Bi = 100$, ... $Bi = 10$)

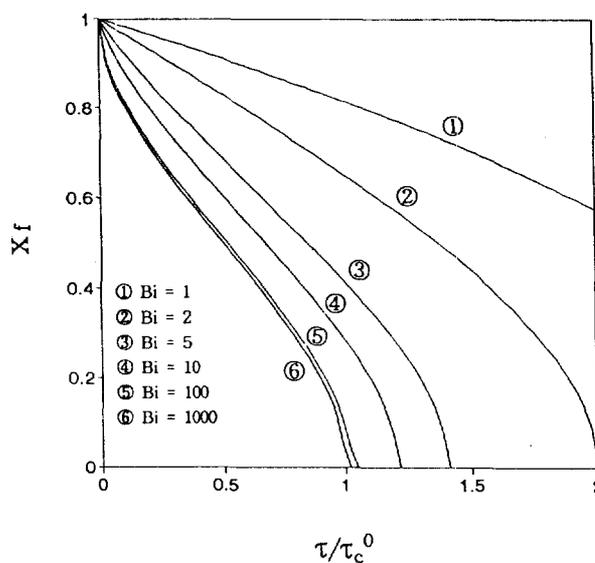


Fig. 4. Effect of Biot number.

able because a large excess amount of regenerant is usually used in most batch regeneration processes. This solution has been applied to the solution of the Shrinking Core Model for gas-solid reactions [11] and the uptake curve of irreversible adsorptions [12].

2. Sensitivity Analysis for Model Parameters

It is very important to check the sensitivity of model parameters on the solution in order to determine the rate-controlling step and the major design variable. Fig. 3 shows the calculated concentration profiles of hydroxide in the resin particle for different values of τ and Bi . When Bi is in the range of 10-100, the film mass transfer resistance could affect the concentration profiles considerably. Fig. 4 shows the effect of Biot number on the variation of the reaction front with respect to the dimensionless time. According to Eq. (33), the dimensionless time necessary

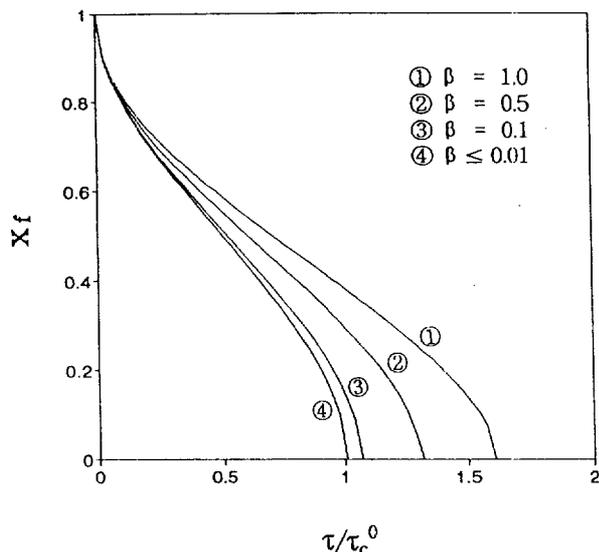


Fig. 5. Effect of β with $Bi=1000$.

to completely regenerate the resin particle is obtained as $1/6$ by letting x_f be equal to zero. It is worthwhile to denote 6τ as τ_c^0 , a reference dimensionless time. τ_c^0 becomes 1.0 for complete regeneration. τ/τ_c^0 means the ratio of the time for complete regeneration to that obtained from the limiting conditions that Bi becomes infinite and β approaches zero, indicating the relative time for complete regeneration. In Figs. 4 and 5, the axis of abscissa is denoted by τ/τ_c^0 for convenience. On the other hand, the left-hand curve in Figs. 4 and 5 with $Bi=\infty$ and $\beta=0$ may be called a "characteristic or reference curve" since it does not change with other operating conditions such as the preloaded amount of phenol and the initial hydroxide concentration. Therefore, Fig. 4 shows clearly the relative effect of Bi on the regeneration process to the reference curve. There is little effect when Bi is greater than 100. In the range of Bi of 10-100, the effect of film mass transfer is considerable as shown in Fig. 3. When Bi is less than 10, pore diffusion is no longer the rate-controlling step. In this case, we have to take into account film mass transfer as well as pore diffusion. It is also interesting to note that the initial slopes, dx_f/dt , in Fig. 4 are proportional to the value of Bi . This fact can be derived from Eq. (28) by assigning x_f as unity,

$$\left(\frac{\partial x_f}{\partial \tau}\right)_{x_f=1} = -Bi \quad (34)$$

It has been known that the regeneration rate is usually influenced by both the film mass transfer and the pore diffusion of hydroxide. Therefore it is a crucial problem to investigate which step controls the overall regeneration rate. We estimated the film mass transfer coefficients of hydroxide as 5×10^{-5} m/s under the shafting rate of 500 rpm [4]. This means that the Biot number is over 100 and the effect of the film mass transfer may be neglected.

The effect of the volume ratio, β , is also investigated. Fig. 5 shows the variation of the reaction front with respect to the value of β . As shown in Fig. 5, the effect of β does not appear when β is less than 0.1. The effect of β can be neglected since typical values of β have been known to be in the range of 10^{-4} - 10^{-2} , in most batch or CSTR adsorbents. However, for fixed-bed regeneration processes, the effect of β should be included in the analy-

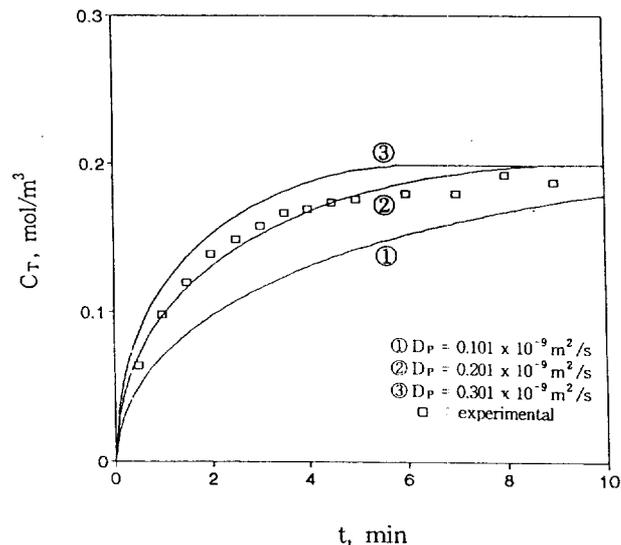


Fig. 6. Determination of effective pore diffusion coefficient, D_p , for Run 2.

($C_s^0=50$ mol/m³, $Q_p=0.35$ mol/kg, $w/V=0.557$ kg/m³, $Bi=100$)

Table 2. Effective pore diffusion coefficients of sodium hydroxide

Run	C_s^0 mol/m ³	w/V kg/m ³	Q_p mol/kg	$D_p \times 10^9$ m ² /s	E %
1	10.0	0.557	0.330	0.340	0.143
2	50.0	0.557	0.350	0.201	0.189
3	100.0	0.557	0.347	0.138	0.218
4	50.0	0.557	0.233	0.177	0.316

sis since the pore space is comparable to the voidage of the column.

3. Determination of Pore Diffusion Coefficients

Now, the remaining question is how to determine effective pore diffusion coefficients of hydroxide from the experimental regeneration data. For this purpose, we can use a minimization routine [13, 14]. In this case, the object function for the routine may be defined as the average root-mean square of differences between calculated and experimental concentrations

$$E = \frac{1}{N} \sum_{i=1}^N \left\{ \frac{\sqrt{(C_{T,exp} - C_{T,cal})^2}}{C_{T,exp}} \right\}_i \quad (35)$$

Fig. 6 shows a typical example for determination of D_p . All values of effective pore diffusion coefficients obtained are listed in Table 2. Effective pore diffusion coefficients of hydroxide during regenerations were determined to be 0.15 - 0.32×10^{-9} m²/s (see Fig. 7). There seems to be a large effect of hydroxide concentration on the effective pore diffusion coefficient. Table 2 shows that D_p is monotonously decreasing with the initial hydroxide concentration. Furthermore, there is a factor of about 2.0 between two diffusion coefficients at 0.01 N and 0.1 N. The molecular diffusion coefficient of sodium hydroxide in an infinite dilute solution at 20°C is 1.83×10^{-9} m²/s [15]. The measured pore diffusion coefficients are considerably smaller than the molecular diffusion coefficient. This implies that the resin particles are highly porous and have a large tortuosity factor [16].

4. Desorption Concentration Curves

Figs. 8 and 9 show the comparisons between predicted and

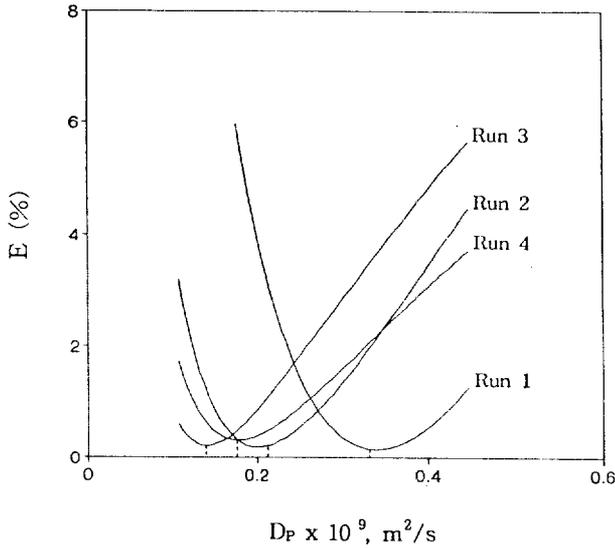


Fig. 7. Minimization results for all runs.

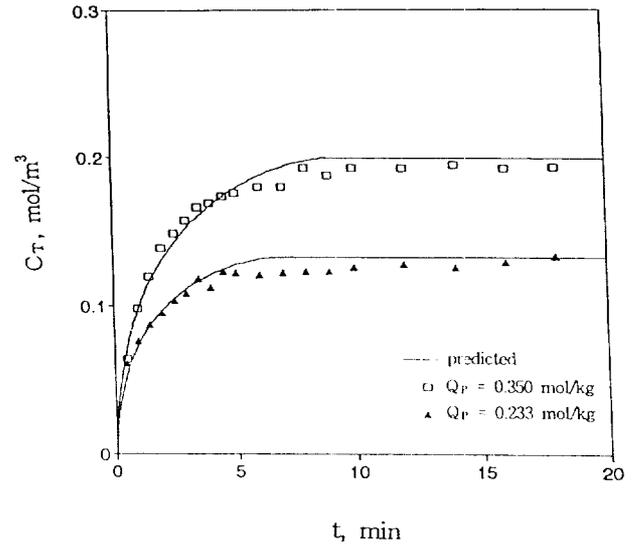


Fig. 9. Regeneration concentration curves with different Q_p (Runs 2 and 4).

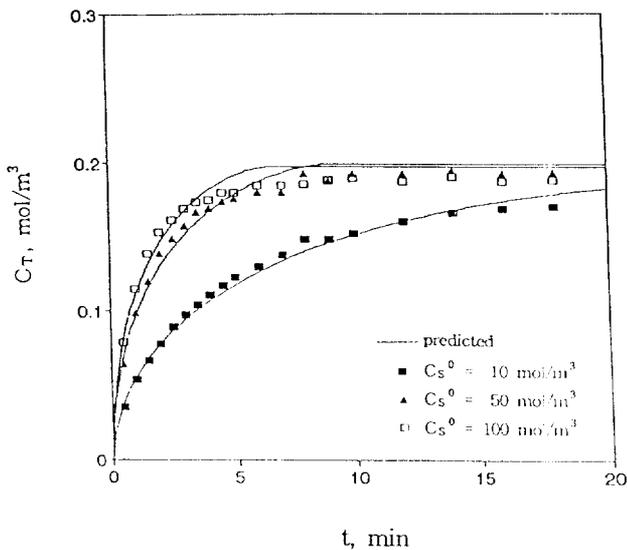


Fig. 8. Regeneration concentration curves with different C_s^0 (Runs 1-3).

measured concentration curves in terms of C_s^0 and Q_p , respectively. These figures represent the effect of the capacity factor, α , on the regeneration curve since α is defined by the ratio of wQ_p to VC_s^0 . The simple model and its analytic solutions simulate satisfactorily the regeneration behavior of SP206 saturated with phenol. Figures also show that most phenol retained by SP206 can be desorbed very quickly within a few minutes even with 0.01 N solution. This implies that the use of polymeric sorbents can be used as an alternative to an activated carbon process for removal of phenol from aqueous solutions.

CONCLUSIONS

From experimental and theoretical works on the regeneration of SP206 which was saturated with phenol, it may be concluded that polymeric sorbents have good properties for, and can be used as an alternative to activated carbons for the removal of phenolic

species from wastewater. The phenol adsorbed on SP206 was desorbed very quickly by sodium hydroxide solutions of 0.01-0.1 N. The simple model, which was developed based on the assumptions of the reaction front and the quasi-steady state profile, successfully simulated general features of the regeneration behavior in a finite adsorber within experimental error. Particularly, analytic solutions of the model are very useful and easy in implementing into most calculations. The model can be later used in simulating a fixed-bed cyclic adsorption operation for removal of phenolic species from wastewater.

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NOMENCLATURE

- b : Langmuir parameter
- B : parameter defined in Eq. (30)
- c_s : concentration of hydroxide inside particle [mol/m³]
- C_s : concentration of hydroxide in batch [mol/m³]
- C_s^0 : initial concentration of hydroxide [mol/m³]
- C_{pN} : molar concentration of phenate [mol/m³]
- C_p : concentration of phenol in batch adsorber [mol/m³]
- C_T : total concentration of phenol and phenate [mol/m³]
- D_p : effective pore diffusion coefficient [m²/s]
- E : average deviation defined in Eq. (35)
- G : parameter defined in Eq. (31)
- H : function of time defined in Eq. (9)
- K_q : reaction equilibrium constant
- k_f : film mass transfer coefficient [m/s]
- Q_p : amount of phenol adsorbed [mol/kg]
- Q_m : amount adsorbed for monolayer formation [mol/kg]
- R : radial position [m]
- R_c : radius of particle [m]
- R_f : reaction front position [m]
- T : temperature [°C]

t : time [s]
 V : volume of solution [m³]
 w : weight of sorbent [kg]
 x, x_r : dimensionless radial coordinates
 Y, y : dimensionless concentrations
 Z : parameter defined in Eq. (32)

Greek Letters

α : capacity factor defined in Eq. (20)
 β : volume ratio defined in Eq. (21)
 ϵ_p : particle porosity
 ρ_p : apparent particle density [kg/m³]
 τ : dimensionless time defined in Eq. (23)

REFERENCES

1. Keith, L. H. and Telliard, W.: *Environ. Sci. Tech.*, **13**, 416 (1979).
2. Garcia, A. A. and King, C. J.: *Ind. Eng. Chem. Res.*, **28**, 204 (1989).
3. Costa, C. and Rodrigues, A.: "Fundamentals of Adsorption", edited by Myers, A. and Belfort, G., 153 (1984).
4. Moon, H., Kook, S. K. and Park, H. C.: *Korean J. Chem. Eng.*, **8**, 168 (1991).
5. Moon, H., Lee, J. W. and Park, H. C.: *Korean J. Chem. Eng.*, **9**, 225 (1992).
6. Costa, C. and Rodrigues, A.: *Chem. Eng. Sci.*, **40**, 707 (1985).
7. Costa, C. and Rodrigues, A.: *AIChE J.*, **31**, 1645 (1985).
8. Costa, C. and Rodrigues, A.: *AIChE J.*, **31**, 1655 (1985).
9. Spahn, H. and Schlunder, E. U.: *Chem. Eng. Sci.*, **30**, 529 (1975).
10. McKay, G. and Bino, M. J.: *Chem. Eng. Res. Des.*, **63**, 168 (1985).
11. Fogler, H. S.: "Elements of Chemical Reaction Engineering", Chap. 10, Prentice-Hall, Englewood Cliffs, 1992.
12. Ruthven, D. M.: "Principles of Adsorption and Adsorption Processes", Chap. 6, John Wiley and Sons, New York, 1984.
13. Moon, H. and Lee, W. K.: *J. Colloid Interface Sci.*, **96**, 162 (1983).
14. Moon, H. and Tien, C.: *Chem. Eng. Sci.*, **43**, 1269 (1988).
15. Reid, R. C., Prausnitz, J. M. and Poling, B. E.: "The Properties of Gases and Liquids", 4th ed., Chap. 11, McGraw-Hill, New York, 1988.
16. Yosida, H., Kataoka, T. and Ikeda, S.: *Can. J. Chem. Eng.*, **63**, 430 (1985).